

Engineering exchange-correlation wave functions, intrinsic Stark effect in quantum well ZnO

Lyubov E Lokot

*V E Lashkaryov Institute of Semiconductor Physics,
Department of Theoretical Physics, Nat. Acad. of Sci. of Ukraine, 41,
Nauky Ave., Kyiv 03028, Ukraine, E-mail address: llokot@gmail.com*

Abstract

In this paper a theoretical studies of the space separation of electron and hole wave functions in the quantum well ZnO/Mg_{0.27}Zn_{0.73}O are presented. For this aim the self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and local exchange-correlation potential is found. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. The shifts of the Hartree valence band spectrums and the conduction band spectrum with respect to the flat band spectrums as well as the Hartree-Fock band spectrums with respect to the Hartree ones are found. An overlap integrals of the wave functions of holes and electron with taking into account besides the piezoelectric effects the exchange-correlation effects in addition is greater than an overlap integral of Hartree ones. The Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that an effective mass of heavy hole of Mg_{0.27}Zn_{0.73}O under biaxial strain is greater than an effective-mass of heavy hole of ZnO. It is calculated that an electron mass is less than a hole mass.

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I. INTRODUCTION

There has been widely studied in the ultraviolet spectral range lasers based on direct wide-bandgap hexagonal würtzite crystal material systems such as ZnO¹⁻⁶. Significant success has been obtained in growth ZnO quantum wells with (ZnMg)O barriers by scrutinized methods of growth^{7,8}. The carrier relaxation from (ZnMg)O barrier layers into a ZnO quantum well through time-resolved photoluminescence spectroscopy is studied in the paper⁹. The time of filling of particles for the single ZnO quantum well is found to be 3 ps⁹.

In the paper we present a theoretical investigation of the intricate interaction of the electron-hole plasma with a polarization-induced electric fields. The confinement of wave functions has a strong influence on the optical properties which is observed with an dependence from the intrinsic electric field which is calculated to be 0.37 MV/cm¹⁰, causing to the quantum-confined Stark effect (QCSE). In this paper we present the results of theoretical studies of the space separation of electron and hole wave functions by self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and the local exchange-correlation potential.

In addition large electron and hole effective masses, large carrier densities in quantum well ZnO are cause for population inversions. These features are comparable to GaN based systems^{11,12}.

An variational simulation in effective-mass approximation is used for the conduction band dispersion and for quantization of holes an Schrödinger equation is solved with würtzite hexagonal effective Hamiltonian¹³ including deformation potentials¹⁴. Keeping in mind the above mentioned equations and the potential energies which have been included in this problem from Poisson's equations we have obtained completely self-consistent band structures and wave functions.

So in this paper we present a self-consistent calculation an above mentioned equations in würtzite ZnO quantum well taking into account the piezoelectric effect and the exchange-correlation potential for bandgap renormalization and engineering of localized Hartree-Fock wave functions. The energy shifts as well as the localization range of exchange-correlational wave functions with respect Hartree energy shifts and Hartree localization range of wave functions require a scrutiny study.

II. THEORY

We take the following wave functions written as vectors in the three-dimensional Bloch space:

$$|\nu \varsigma_v k_t\rangle = \begin{pmatrix} \sum_{i=1}^m \Psi_{k_t}^{(1)}[i, \nu] \psi_i(Z) \\ \sum_{i=1}^m \Psi_{k_t}^{(2)}[i, \nu] \psi_i(Z) \\ \sum_{i=1}^m \Psi_{k_t}^{(3)}[i, \nu] \psi_i(Z) \end{pmatrix} \begin{pmatrix} |1, \varsigma_v\rangle \\ |2, \varsigma_v\rangle \\ |3, \varsigma_v\rangle \end{pmatrix}. \quad (1)$$

The Bloch vector of ν -type hole with spin $\varsigma_v = \pm$ and momentum k_t is specified by its three coordinates $[\Psi_{k_t}^{(1)}[m, \nu], \Psi_{k_t}^{(2)}[m, \nu], \Psi_{k_t}^{(3)}[m, \nu]]$ in the basis $[|1, \varsigma_v\rangle, |2, \varsigma_v\rangle, |3, \varsigma_v\rangle]$ ¹⁵, known as spherical harmonics with the orbital angular momentum $l = 1$ and the eigenvalue m_l its z component. The envelope Z -dependent part of the quantum well eigenfunctions can be specified from the boundary conditions $\psi_m(Z = 0) = \psi_m(Z = 1) = 0$ of the infinite quantum well as

$$\psi_m(Z) = \sqrt{\frac{2}{w}} \sin(\pi m Z), \quad (2)$$

where $Z = (\frac{z}{w} + \frac{1}{2})$, m is a natural number. Thus the hole wave function can be written as

$$\Psi_{\nu \varsigma_v k_t}(\mathbf{r}) = \frac{e^{i k_t \rho_t}}{\sqrt{A}} |\nu \varsigma_v k_t\rangle. \quad (3)$$

The valence subband structure $E_\nu^{\varsigma_v}(k_t)$ can be determined by solving equations system:

$$\begin{aligned} \sum_{j=1}^3 (H_{ij}^{\varsigma_v}(k_z = -i \frac{\partial}{\partial z}) + V(z) + \delta_{ij} E_\nu^{\varsigma_v}(k_t)) \times \\ \times \phi_\nu^{(j)\varsigma_v}(z, k_t) = 0, \end{aligned} \quad (4)$$

where $i = 1, 2, 3$.

The wave function of electron of first energy level with accounts QCSE¹⁶:

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{A}} e^{i k_t \rho} \Psi(Z, \xi) |S\rangle |\varsigma_c\rangle, \quad (5)$$

where

$$\Psi(Z, \xi) = \begin{cases} \psi_1(Z, \xi) = C_1 e^{(\kappa_0 - \xi)(wZ)}, Z \in (-\infty..0) \\ \psi(Z, \xi) = C \sin(k_0 w (Z - \frac{1}{2}) + \delta_0) e^{-\xi w (Z - \frac{1}{2})}, Z \in [0..1] \\ \psi_2(Z, \xi) = C_2 e^{-(\kappa_0 + \xi)w(Z-1)}, Z \in (1..\infty). \end{cases} \quad (6)$$

From bond conditions^{16,17} $\psi_1(Z, \xi)|_{Z=0} = \psi(Z, \xi)|_{Z=0}$, $\psi_2(Z, \xi)|_{Z=1} = \psi(Z, \xi)|_{Z=1}$, $\frac{\psi_1'(Z, \xi)}{\psi_1(Z, \xi)}|_{Z=0} = \frac{\psi'(Z, \xi)}{\psi(Z, \xi)}|_{Z=0}$, $\frac{\psi_2'(Z, \xi)}{\psi_2(Z, \xi)}|_{Z=1} = \frac{\psi'(Z, \xi)}{\psi(Z, \xi)}|_{Z=1}$, one can find $C_1 = C \sin(-\frac{k_0 w}{2} + \delta_0) e^{\xi \frac{w}{2}}$,

$C_2 = C \sin(\frac{k_0 w}{2} + \delta_0) e^{-\xi \frac{w}{2}}$, $\kappa_0 = k_0(\frac{1 - \cos k_0 w}{\sin k_0 w})$, $\delta_0 = \frac{k_0 w}{2} + \arctan \frac{\kappa_0}{k_0}$, where A is the area of the quantum well in the xy plane, ρ is the two-dimensional vector in the xy plane, $k_t = (k_x, k_y)$ is in-plane wave vector. The constant multiplier C is found from normalization condition:

$$\int_{-\infty}^{\infty} |\Psi(Z, \xi)|^2 w dZ = 1. \quad (7)$$

One can find the functional, which is built in the form:

$$J(\xi) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad (8)$$

where

$$H = H_c + V(z), \quad (9)$$

where H_c is a conduction band kinetic energy including deformation potential.

From Kane model one can define the band-edge parameters such as the crystal-field splitting energy Δ_{cr} , the spin-orbit splitting energy Δ_{so} and the momentum-matrix elements for the longitudinal ($\mathbf{e} \parallel z$) z-polarization and the transverse ($\mathbf{e} \perp z$) polarization : $P_z \equiv \langle S | \hat{p}_z | Z \rangle$, $P_{\perp} \equiv \langle S | \hat{p}_x | X \rangle \equiv \langle S | \hat{p}_y | Y \rangle$. Here we use the effective-mass parameters, energy splitting parameters, deformation potential parameters as in papers ^{14,20,21}.

The potential energies $V(z)$ can be looked for as follows:

$$V(z) = e\Phi^H(z) + \delta U_{c,v}(z) + \Phi_{xc}(z), \quad (10)$$

where $\Phi^H(z)$ is the solution of one-dimensional Poisson's equation with the strain-induced electric field in the quantum well, $\delta U_{c,v}(z)$ are the conduction and valence band edge discontinuities which can be represented in the form ¹⁸:

$$\delta U_c(z) = \begin{cases} U_0 - eEw(\frac{z}{w} + 1), & z \in (-\infty.. -w/2) \\ eEz, & z \in [-w/2..w/2] \\ U_0 - eEw(\frac{z}{w} - 1), & z \in (w/2..\infty). \end{cases} \quad (11)$$

$\Phi_{xc}(z)$ is exchange-correlation potential energy which is found from the solution three-dimensional Poisson's equation, using both an expression by Gunnarsson and Lundquist ¹⁹, and following criterions. At carrier densities $4 * 10^{12} \text{ cm}^{-2}$, $k_F > \sqrt{n}/4$ at a temperature $T=0 \text{ K}$ as $1 > 0.1$ has been carried. k_F is Fermi wave vector. The criterion is independent from a width of well. The solution of equations system (4), (8), (11), (12) as well as (4), (8),

(10), (23) is independent from a temperature. The ratio of Coulomb potential energy to the Fermi energy is $r_s = E_C/E_F = 0.63 < 1$. The problem consists of the one-dimensional Poisson's equation solving of which may be found Hartree potential energy and three-dimensional Poisson's equation which separated on one-dimensional and two-dimensional equations by separated of variables using an criterion $[\Psi_{\alpha,\nu,n}(k_F, z) \sin \mathbf{k}_F \boldsymbol{\rho}] \ll 1$, where $\alpha = e, h$. The three-dimensional Poisson's equation includes local exchange-correlation potential:

$$\frac{d^2 \Phi_{e,h}^H}{dz^2} = \frac{4\pi}{\kappa} \rho_{e,h}^H(z; g), \quad (12)$$

$$\Delta_\rho \Phi_{e,h}^{xc} = \frac{4\pi}{\kappa} \rho_{e,h}^{xc}(\mathbf{r}, \mathbf{r}'), \quad (13)$$

where

$$\rho_{e,h}^H(z; g) = \mp e \sum_{\alpha, n, k_t} |\Psi_{e,h,\alpha,n}(k_t, z)|^2 f_{n,\alpha}(k_t; g), \quad (14)$$

$$\begin{aligned} f_n(k_t; g) &= \frac{1}{e^{(\epsilon_{n,k_t} + \frac{g}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \mu)/kT} + 1}} = \\ &= \frac{1}{(e^{1(1+r_s+r_s^2+\dots)})^{(\epsilon_{n,k_t} - \mu)/kT} + 1}}. \end{aligned} \quad (15)$$

Solving one-dimensional Poisson's equation (12) one can find screening polarization field and Hartree potential energy which is substituted in the Schrödinger equations from which are found wave functions and bandstructure. The conclusive determination of screening polarization field is determined by iterating Eqs. (4), (8), (11), (12) until the solutions of conduction and valence band energies and wave functions are converged:

$$\Phi^H(z) = \Phi_h^H(z) + \Phi_e^H(z), \quad (16)$$

$$\begin{aligned} e\Phi_h^H(z) &= \frac{2e^2}{\kappa} \sum_{\nu, n, k, i} g_\nu \int k_t dk_t \langle v_i, \varsigma_\nu | \Psi_{k_t}^i[\nu, m] \Psi_{k_t}^i[\nu, l] | \varsigma_\nu, v_i \rangle f_{\nu,p}(k_t) \times \\ &\times \begin{cases} w \left(\frac{\cos \pi (\frac{z}{w} + \frac{1}{2})(l+m)}{\pi^2(l+m)^2} - \frac{\cos \pi (\frac{z}{w} + \frac{1}{2})(m-l)}{\pi^2(m-l)^2} \right), m \neq l \\ w \left(\frac{(\frac{z}{w} + \frac{1}{2})^2}{2} + \frac{1}{4} \frac{\cos 2\pi m (\frac{z}{w} + \frac{1}{2})}{\pi^2 m^2} \right), m = l, \end{cases} \end{aligned} \quad (17)$$

$$\begin{aligned} e\Phi_e^H(z) &= -\frac{2e^2}{\kappa} g_1 \int k_t dk_t C^2 f_{1n}(k_t) \times \\ &\times \begin{cases} \frac{1 - \cos(-k_0 w + 2\delta_0)}{2} e^{\xi w} \frac{e^{2(\kappa_0 - \xi)(z + \frac{w}{2})}}{4(\kappa_0 - \xi)^2}, z \in (-\infty.. -w/2) \\ \frac{e^{-2\xi z}}{8\xi^2} - \frac{2 \cos 2(k_0 z + \delta_0) e^{-2\xi z}}{(4\xi^2 + 4k_0^2)^2} (\xi^2 - k_0^2) + \frac{\sin 2(k_0 z + \delta_0) e^{-2\xi z}}{4(\xi^2 + k_0^2)^2} k_0 \xi, z \in [-w/2..w/2] \\ \frac{1 - \cos(k_0 w + 2\delta_0)}{2} e^{-\xi w} \frac{e^{-2(\kappa_0 + \xi)(z - \frac{w}{2})}}{4(\kappa_0 + \xi)^2}, z \in (w/2.. \infty), \end{cases} \end{aligned} \quad (18)$$

where $Z = \frac{z}{w} + \frac{1}{2}$, g_ν and g_1 correspond to the degeneration of the ν hole band and the first quantized conduction band, respectively, e is the value of electron charge, κ is the permittivity of a host material, and $f_{\nu,p}(k_t)$, $f_{1n}(k_t)$ are the Fermi-Dirac distributions for holes and electrons.

Exchange-correlation charge density may be determined as:

$$\begin{aligned} \rho_{e,h}^{xc}(\mathbf{r}, \mathbf{r}') = \\ = \sum_{l=0}^{\infty} \sum_{m=-l}^l |\Psi_{e,h,\alpha,n}(k_t, z)|^2 \rho_{lm}(\boldsymbol{\rho} - \boldsymbol{\rho}') Y_{lm}\left(\frac{\boldsymbol{\rho} - \boldsymbol{\rho}'}{|\boldsymbol{\rho} - \boldsymbol{\rho}'|}\right), \end{aligned} \quad (19)$$

using the expansion of plane wave

$$\begin{aligned} \sum_{l=0}^{\infty} \sum_{m=-l}^l \rho_{lm}(\boldsymbol{\rho}) Y_{lm}\left(\frac{\boldsymbol{\rho}}{|\boldsymbol{\rho}|}\right) = \\ = e^{i \mathbf{k}_t \boldsymbol{\rho}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l j_l(\mathbf{k}_t \boldsymbol{\rho}) Y_{lm}^*\left(\frac{\mathbf{k}_t}{k_t}\right) Y_{lm}\left(\frac{\boldsymbol{\rho}}{|\boldsymbol{\rho}|}\right). \end{aligned} \quad (20)$$

At the condition $[\Psi_{\alpha,\nu,n}(k_F, z) \sin \mathbf{k}_F \boldsymbol{\rho}] \ll 1$, the solution eq. (13) may be found as follows

$$\Phi_{e,h}(xc) = \int_0^\infty \rho \rho_{00}(\boldsymbol{\rho}) \frac{1}{\rho} d\rho. \quad (21)$$

The solution the three-dimensional Poisson's equation may be presented in the form:

$$\Phi_{e,h}^{xc}(z) = \Phi_{e,h}^H(z) \Phi_{e,h}(xc). \quad (22)$$

The complete potential which describes piezoelectric effects and local exchange-correlation potential in quantum well one can find as follows

$$\Phi(z) = \Phi_h^H(z) + \Phi_e^H(z) + \Phi_h^H(z) \Phi_h(xc) + \Phi_e^H(z) \Phi_e(xc). \quad (23)$$

III. RESULTS AND DISCUSSIONS

We consider QCSE in strained würtzite ZnO/Mg_{0.27}Zn_{0.73}O quantum well with width 4 nm, in which the barrier height is a constant value for electrons and is equal to $U_0 = 536.22$ meV. The theoretical analysis of piezoelectric effects and exchange-correlation effects is based on the self-consistent solution of the Schrödinger equations for electrons and holes in quantum well of width w with including Stark effect and the Poisson equations. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density

for electrons and holes along the polarization field distribution the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. All calculations are performed at a temperature of 300 K. The transverse components of the biaxial strain are proportional to the difference between the lattice constants of materials of the well and the barrier and depend on the Mg content x : $\epsilon_{xx} = \epsilon_{yy} = \frac{a_{Mg_xZn_{1-x}O} - a_{ZnO}}{a_{ZnO}}$, $a_{Mg_xZn_{1-x}O} = a_{ZnO} + x(a_{MgO} - a_{ZnO})$, $a_{ZnO} = 0.32496$ nm, $a_{MgO} = 0.4216$ nm²¹. The longitudinal component of a deformation is expressed through elastic constants and the transverse component of a deformation: $\epsilon_{zz} = -2\frac{C_{13}}{C_{33}}\epsilon_{xx}$.

The physical parameters for ZnO can be looked as follows. We take the effective-mass parameters²⁰: $A_1 = -2.743$, $A_2 = -0.393$, $A_3 = 2.377$, $A_4 = -2.069$, $A_5 = -2.051$, $A_6 = -2.099$, $m_e^\perp = 0.329$ the parameters for deformation potential¹⁴: $D_1 = -3800$ meV, $D_2 = -3800$ meV, $D_3 = -800$ meV, $D_4 = 1400$ meV, $D_{cz} := -6860$ meV, $D_{c\perp} := -6260$ meV, and the energy parameters at 300 K^{20,21}: $E_g = 3400$ meV, $\Delta_1 = \Delta_{cr} = 36.3$ meV, $\Delta_2/3 = 0.63$ meV, $\Delta_3/3 = 2.47$ meV, the elastic constant²¹: $C_{13} = 90$ GPa and $C_{33} = 196$ GPa, the permittivity of the host materials $\kappa = 7.8$.

We have calculated carriers population of the lowest conduction band and the both heavy hole and light hole valence band. Solving (4) for holes in the infinitely deep quantum well and finding the minimum of functional (8) for electrons in a quantum well with barriers of finite height, we can find the energy and wave functions of electrons and holes with respect Hartree potential and exchange-correlational potential in a piezoelectric field at a carriers concentration $n = p = 4 * 10^{12}$ cm⁻². The screening field is determined by iterating Eqs. (4), (8), (10), (23) until the solution of energy spectrum is converged.

The dispersion of the renormalization band gap is presented in Fig. 6. We have compared the Hartree band gap with the flat band gap as well as the Hartree band gap with the Hartree-Fock band gap and have found $E_g^H - E_g^{Flatband} = 20.72$ meV, $E_g^{HF} - E_g^H = 4.40$ meV. Comparing E_g^{HF} and E_g^H and a form of bedplate of quantum well for electrons which is presented in Fig. 3 as well as an even form of bedplate of quantum well for holes one can see that an electron mass is less than a hole mass. The effective masses $Mg_{0.27}Zn_{0.73}O$ under biaxial strain for the heavy holes and light holes are presented in Fig. 1. Comparing the effective mass of $Mg_{0.27}Zn_{0.73}O$ under biaxial strain for the heavy hole with the effective mass of $Al_{0.3}Ga_{0.7}N$ under biaxial strain for the heavy hole which is presented in Fig. 2 one can see that a mass of heavy hole of $Mg_{0.27}Zn_{0.73}O$ is greater than a mass of heavy hole

of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$. Comparing the effective mass of $\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ under biaxial strain for the heavy hole with an effective-mass parameter $A_1 = -2.743$ one can conclude that an effective mass of heavy hole of $\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ under biaxial strain is greater than an effective-mass of heavy hole of ZnO .

The Hartree and Hartree-Fock wave functions for electrons, heavy holes and light holes are presented in Fig. 4. From Fig. 4 one can conclude that an overlap integrals of the wave functions of holes and electron with taking into the account besides the piezoelectric effects the exchange-correlation effects in addition are greater than an overlap integrals of Hartree ones. Hartree charge density distribution and Hartree-Fock charge density distribution are presented in Fig. 5. Comparing charge density distributions presented in Fig. 5 one can conclude that Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles.

IV. CONCLUSIONS

In this paper a theoretical studies of the space separation of electron and hole wave functions in the quantum well $\text{ZnO}/\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ by the self-consistent solution of the Schrödinger equations for electrons and holes and the Poisson equations at the presence of spatially varying quantum well potential due to the piezoelectric effect and local exchange-correlation potential are presented. The exchange-correlation potential energy is found from the solution three-dimensional Poisson's equation, using both an expression by Gunnarsson and Lundquist¹⁹, and following criterions. At carrier densities $4 * 10^{12} \text{ cm}^{-2}$, $k_F > \sqrt{n}/4$ at a temperature $T=0 \text{ K}$ as $1 > 0.1$ has been carried. The criterion is independent from a width of well. The solution of equations system (4), (8), (11), (12) as well as (4), (8), (10), (23) is independent from a temperature. The ratio of Coulomb potential energy to the Fermi energy is $r_s = E_C/E_F = 0.63 < 1$. The one-dimensional Poisson equation contains the Hartree potential which includes the one-dimensional charge density for electrons and holes along the polarization field distribution. The three-dimensional Poisson equation contains besides the one-dimensional charge density for electrons and holes along the polarization field distribution the exchange-correlation potential which is built on convolutions of a plane-wave part of wave functions in addition. The problem consists of the one-dimensional Poisson's equation solving of which may be found Hartree potential energy and three-dimensional

Poisson's equation which separated on one-dimensional and two-dimensional equations by separated of variables, at the condition that the ratio of wave function localization in the longitudinal z direction on transversal in-plane wave function localization is less 1. We have compared the Hartree band gap with the flat band gap as well as the Hartree band gap with the Hartree-Fock band gap and have found $E_g^H - E_g^{Flatband} = 20.72$ meV, $E_g^{HF} - E_g^H = 4.40$ meV. An overlap integrals of the wave functions of holes and electron with taking into account besides the piezoelectric effects the exchange-correlation effects in addition is greater than an overlap integral of Hartree ones. The Hartree particles distribute greater on edges of quantum well than Hartree-Fock particles. It is found that an effective mass of heavy hole of $\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ under biaxial strain is greater than a effective-mass of heavy hole of ZnO . It is calculated that an electron mass is less than a hole mass.

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Figure captions

FIG. 1. The transverse effective masses for $\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ under biaxial strain: (a) for the heavy hole; (b) for the light hole.

FIG. 2. The transverse effective masses for $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ under biaxial strain: (a) for the heavy hole; (b) for the light hole.

FIG. 3. For the quantum well $\text{ZnO}/\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ with a width 4nm, at a carriers concentration $4 \times 10^{12} \text{ cm}^{-2}$, at a temperature 300 K: (a) Hartree screening potential; (b) Hartree-Fock screening potential.

FIG. 4. For the quantum well $\text{ZnO}/\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ with a width 4nm, at a carriers concentration $4 \times 10^{12} \text{ cm}^{-2}$, at a temperature 300 K, at a transverse wave vector $k_t = 2 \times 10^7 \text{ cm}^{-1}$: (a) Hartree wave functions; (b) Hartree-Fock wave functions.

FIG. 5. For the quantum well $\text{ZnO}/\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ with a width 4nm, at a carriers concentration $4 \times 10^{12} \text{ cm}^{-2}$, at a temperature 300 K: (a) Hartree charge density; (b) Hartree-Fock charge density.

FIG. 6. For the quantum well $\text{ZnO}/\text{Mg}_{0.27}\text{Zn}_{0.73}\text{O}$ with a width 4nm, at a carriers concentration $4 \times 10^{12} \text{ cm}^{-2}$, at a temperature 300 K: (a) conduction band energy; (b) valence band energy.

Figures

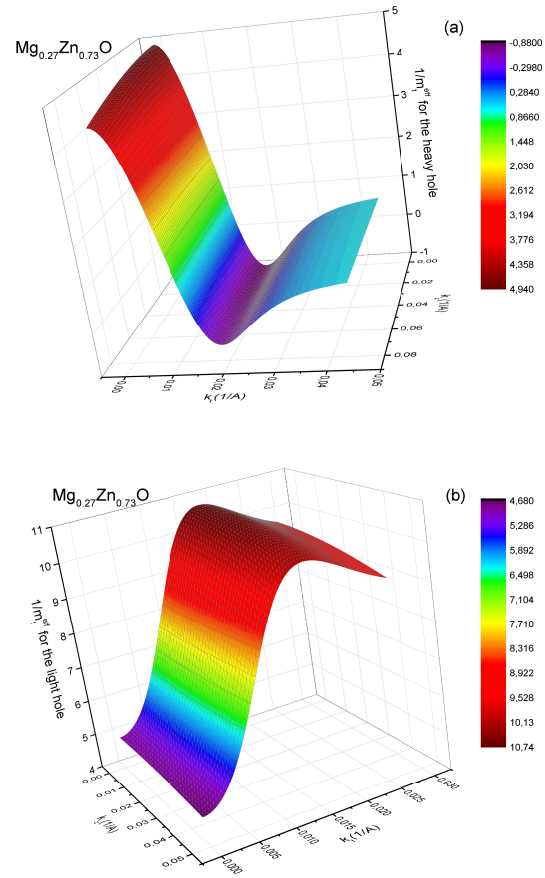


FIG. 1:

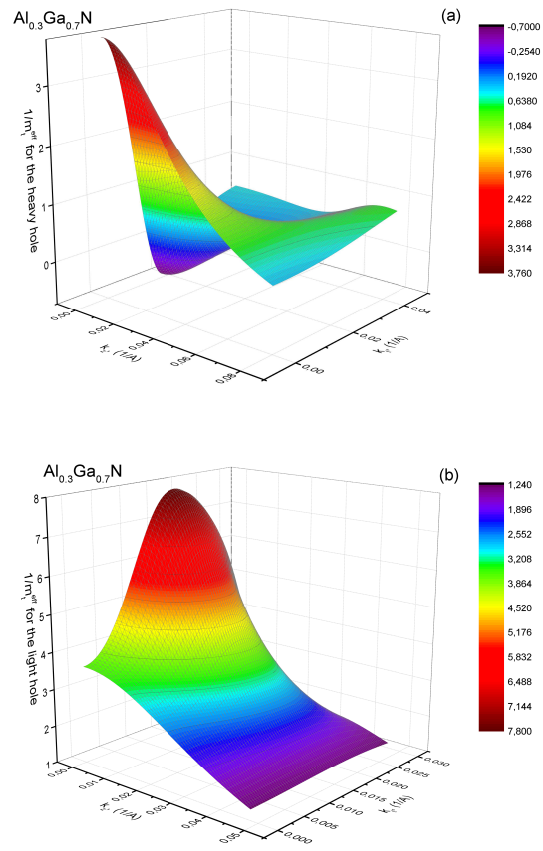


FIG. 2:

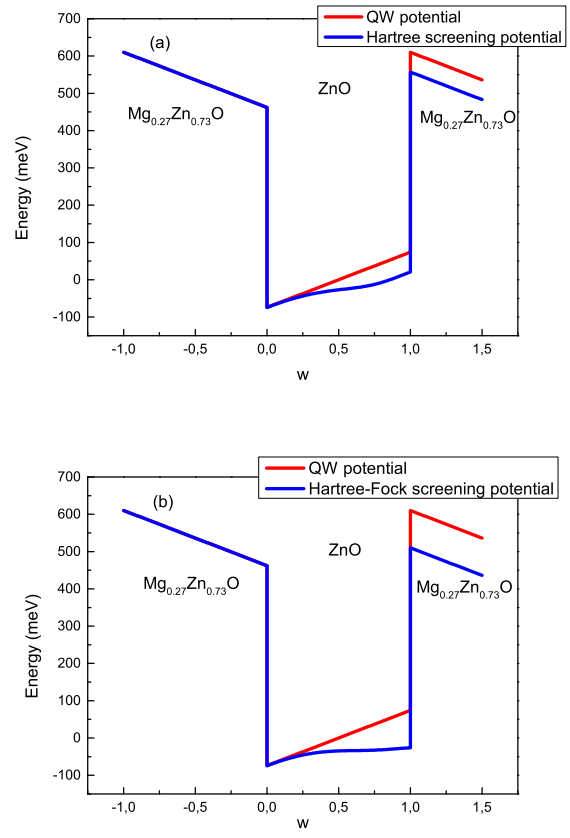


FIG. 3:

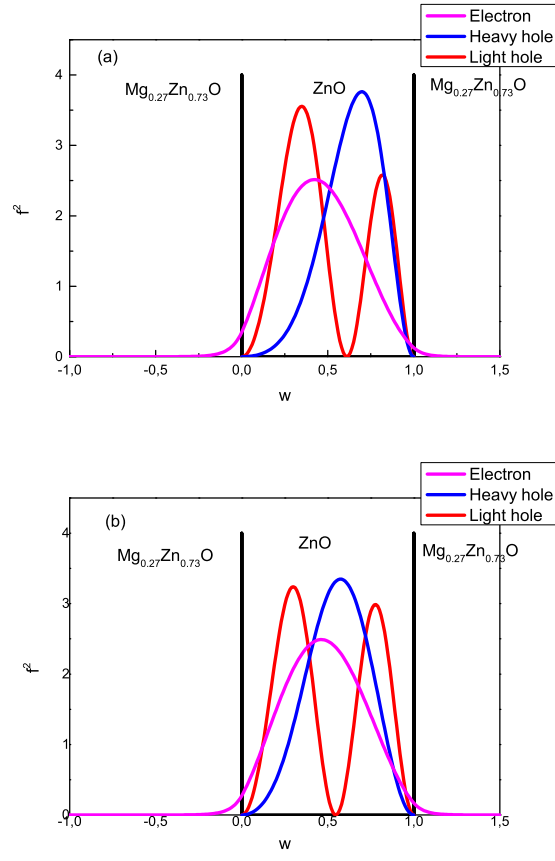


FIG. 4:

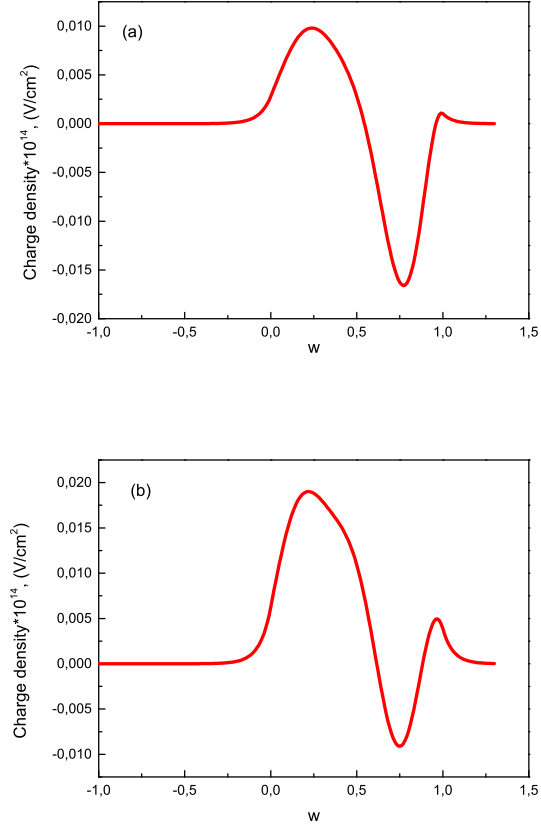


FIG. 5:

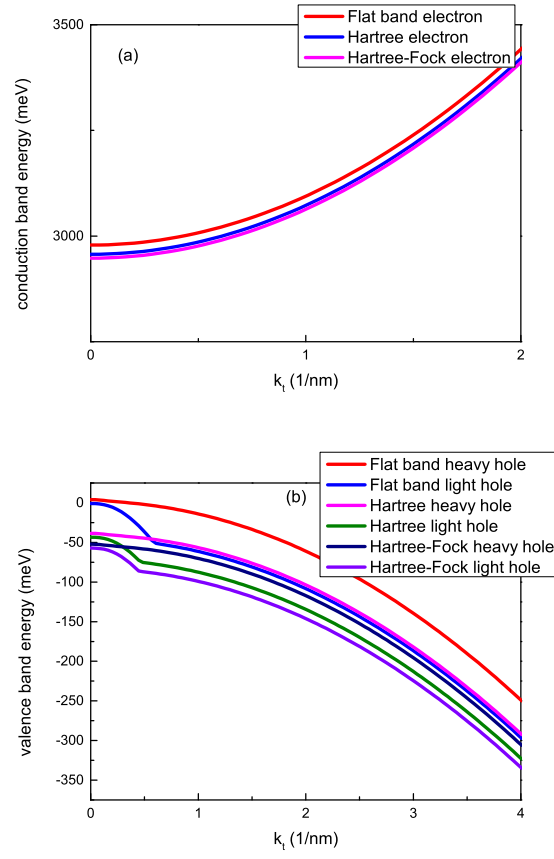


FIG. 6: